Kinetics of the Phase Separation Transition in Cold-Atom Boson-Fermion Mixtures

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We study the kinetics of the first order phase separation transition in boson-fermion cold-atom mixtures. At sufficiently low temperatures such a transition is driven by quantum fluctuations responsible for the formation of critical nuclei of a stable phase. Based on a microscopic description of interacting boson-fermion mixtures we derive an effective action for the critical droplet and obtain an asymptotic expression for the nucleation rate in the vicinity of the phase transition and near the spinodal instability of the mixed phase. We also discuss effects of dissipation which play a dominant role close to the transition point, and identify the regimes where quantum nucleation can be experimentally observed in cold-atom systems.

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Kinetics of the first order phase transitions at ultralow temperatures has received considerable attention in connection with several problems ranging from the decay of false vacuum in field theoretical models of the early Universe [1] to the phase separation in ^{3}He-^{4}He mixtures [2]. In the latter case it has been argued that below a certain temperature (of the order of a few tens of mK) formation of pure ^{3}He phase from a supersaturated mixture occurs via the process of quantum nucleation, where critical nuclei overcome the potential barrier (due to the surface energy between the two phases) by means of quantum tunneling. It has been predicted theoretically [3] that the rate of such nucleation behaves as $\exp\left(-C/\Delta\mu^{7/2}\right)$, where $\Delta\mu$ is the degree of supersaturation, i.e., the difference in chemical potentials of the two phases, and C is related to the coefficients of the phenomenological Ginzburg-Landau expansion of the free energy near the point of the phase transition. Measurements carried out by several groups [4] seem to confirm that at sufficiently low temperatures the kinetics of the phase separation in ^{3}He-^{4}He becomes temperature independent; however, they have been unable to verify the expected dependence of the nucleation rate on the systems' parameters (i.e., $\Delta\mu$, etc) - partly due to the poor knowledge of microscopic interactions between particles in such a strongly correlated system.

We argue that contemporary cold atom systems provide a perfect setup for studying and observing the kinetics of such a phase separation transition. Atomic mixtures, such as boson-fermion mixture, are commonly realized in experiments on sympathetic cooling, where one of the species (typically bosons) plays the role of a coolant [5]. Another interesting realization of boson-fermion mixture has been demonstrated in a two-component fermion system, where strongly bound Cooper pairs correspond to bosons interacting with unpaired fermion atoms [6]. Starting from a microscopic description of a boson-fermion mixture we derive an effective action for the order parameter (the condensate density) taking into account fermion-boson interaction. We show explicitly that the classical potential for the order parameter due to such interaction has two minima corresponding to the two phases of the system (mixed and phase separated). The two minima are separated by the finite energy barrier, which points out that such a transition is indeed of the first order [7]. We then derive an expression for the nucleation (tunneling) rate of the critical droplet of the pure fermion phase near the phase transition line and near the line of absolute (spinodal) instability of the mixed phase. We also evaluate the role of dissipation [8] in the quantum nucleation process and find that near the line of the first order phase transition it changes the leading asymptotic behavior of the nucleation rate on the degree of supersaturation.

We consider a Bose-Einstein condensate interacting with a single species of fermions (in the same spin state). Interactions in such a mixture are characterized by two scattering lengths a_{BB} and a_{BF}. Fermions and bosons interact through contact potential $\lambda_{BF}\delta(\mathbf{r}-\mathbf{r'})$, contributing term $\lambda_{BF}\rho\psi_F^\dagger\psi_F$, where $\lambda_{BF} = 2\pi\hbar^2 a_{BF}(1/m_B+1/m_F)$; $\sqrt{\rho}e^{i\phi}$ and ψ_F are bosonic and fermionic fields respectively. In addition, boson-boson interaction gives rise to another term $\lambda_{BB}\rho^2/2$ in the Hamiltonian density, with $\lambda_{BB} = 4\pi\hbar^2 a_{BB}/m_B$. The direct coupling between fermions is negligible due to the exclusion principle in the s-scattering channel (p-wave scattering is usually small compared to s-wave fermion-boson and boson-boson interactions). For the purposes of present calculation we can neglect the spatial dependence of the trapping potential and assume that the local densities of fermions and bosons are set by the chemical potentials μ_F and μ_B. Indeed, since the first order transition occurs at finite coherence length (to be defined below), the shape of the trap potential should play little role in the dynamics of the phase transition as long

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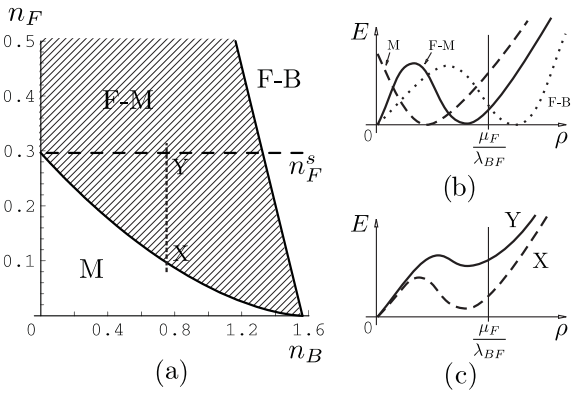

FIG. 1: (a) The phase diagram of the equilibrium boson-fermionic mixture. The bosonic density n_B is in units of $\frac{9\pi}{4}(a_{BB}^2/a_{BF}^5)(m_F^2/m_B^2)\,(m_F/m_B+1)^{-5}$ and the fermionic density n_F is in units of $\frac{9\pi}{2}(a_{BB}^3/a_{BF}^6)(m_F^3/m_B^3)$ $\times\,(m_F/m_B+1)^{-6}$. The area where pure fermionic fraction can coexist with the mixture (F-M) is hatched. The mixture is unstable above the dashed line. (b) Three possible curves for $E(\rho)$ at equilibrium (sketch). (c) The sketch of $E(\rho)$ for out-of-equilibrium mixture: above the lower phase separation curve (dashed curve) and below the instability line (solid curve). The corresponding points are shown on the phase diagram (a).

as the effective size of the trap is much greater than the coherence length.

It is convenient to describe the system in terms of the bosonic field only, averaging e^{-H/k_BT} (H is the overall Hamiltonian) with respect to the fermionic field. Such averaging can be easily carried out within mean field, i.e., the Thomas-Fermi approximation [9, 10], so that the calculation reduces to the evaluation of the canonical partition function (or free energy) of the free fermions with effective chemical potential $\mu_F-\lambda_{BF}\rho$. In the zero-temperature limit the effective classical potential density for the bosons is

$$E(\rho)= -\mu_B\rho+\frac{1}{2}\lambda_{BB}\rho^2 - \frac{(2m_F)^{3/2}}{15\pi^2\hbar^3}\,(\mu_F-\lambda_{BF}\rho)^{5/2}\,\theta(\mu_F-\lambda_{BF}\rho), \quad (1)$$

where $\theta(x)$ is a step function. It is known that a fermion-boson mixture with pointlike interactions exhibits three different phases [9]: uniform mixture of bosons and fermions (M), pure fermion fraction coexisting with the mixture (F-M), and separated bosonic and fermionic fractions (F-B), see Fig 1a. Equation (1) is sufficient to obtain the entire structure of the phase diagram. Indeed, one can notice that $E(\rho)$ has either one or two local minima separated by the barrier (see Fig. 1b). The one at $\rho=0$ corresponds to pure fermionic phase. The other, $\rho=\rho_0$, characterizes the mixture if $\rho_0<\mu_F/\lambda_{BF}$, or pure bosons, if $\rho_0\geq\mu_F/\lambda_{BF}$. At low densities only the mixture exists at equilibrium. For higher densities the mixture becomes metastable and, eventually, unstable above the absolute (spinodal) instability line. The phase transition line between M and F-M phases can be obtained from the condition $E(0)=E(\rho_0)$ in Eq. (1) in the parametric form: $n_F^0=A^{-3}y^3/8$, $n_B^0=A^{-2}[1-y^2]/4$, where the densities are in the units of Fig. 1a, $A=3\pi^2\hbar^3\lambda_{BB}/(2m_F)^{3/2}\lambda_{BF}^2\mu_F^{1/2}$, and parameter y is obtained from the equation $2+4y+6y^2+3y^3-5A(1+y)^2=0$. Note that the solution with $0<y<1$ exists only for $2/5\leq A\leq 3/4$.

In what follows we consider the system with fixed global density of the bosons n_B. Upon variation of fermion density in the metastable region, i.e., between points X and Y in Fig. 1a, the classical potential $E(\rho)$ varies continuously between the two situations shown schematically in Fig. 1c: with nearly equal minima in the vicinity of the phase transition point (at $n_F=n_F^0+\Delta n_F$) and vanishingly small barrier near the absolute instability at $n_F=n_F^s=8/27$ (in dimensionless units). In the rest of this Letter we study kinetics of the system, i.e., the rate of formation of the stable pure fermion phase out of the metastable mixed phase in these two limiting cases. To do so we consider an effective Lagrangian density of the bosons, which can be written in density-phase variables as

$$L=\hbar\rho\dot{\phi}+\frac{\hbar^2}{2m_B}\rho(\nabla\phi)^2+\frac{\hbar^2}{8m_B\rho}(\nabla\rho)^2+E(\rho). \quad (2)$$

The first term in Eq. (2) is the Berry phase term, while the second and the third terms are the kinetic energy of the superfluid. The Thomas-Fermi approximation utilized in Eqs. (1,2) implies that renormalization of the boson kinetic energy arising due to the non-locality of the fermionic response function is relatively small. A straightforward perturbative estimate (to the second order in λ_{BF}) yields the gradient term, i.e. the correction to the Thomas-Fermi, $\sim (m_F^{3/2}\lambda_{BF}^2\mu_F^{1/2}/\hbar^3k_F^2)(\nabla\rho)^2$. Comparing this term with the third term in Eq. (2) we see that near the phase transition line it is smaller by factor $\sim (k_Fl)^{-2}$, where l is boson coherence length, $l\sim a_{BB}/g_B$, and $g_B^2=a_{BB}^3\rho_0$ is conventional boson gas parameter, which, in terms of the dimensionless n_B (as in Fig.1) is

$$g_B^2=\frac{9\pi}{4}\left(\frac{a_{BB}}{a_{BF}}\right)^5\left(\frac{m_F}{m_B}\right)^2\left(\frac{m_F}{m_B}+1\right)^{-5}n_B.$$

For $g_B\lesssim 0.1$ and not too small n_F (e.g. for $n_B\sim 0.4$), $(k_Fl)^2\sim 50$, and thus the Thomas-Fermi approximation is well justified.

The decay rate per unit volume (Γ/V) from a metastable state (at ρ_0) can be obtained by calculating the classical action for the transition between states with $\rho=\rho_0$ and $\rho=0$ in the imaginary time formalism by following the prescription of Ref. [1]. Namely, $\Gamma/V\sim\exp(-S/\hbar)$, where the action $S=\int dtd\mathbf{r}L(\rho,\phi)$

is evaluated over the classical (extremal) trajectory, defined by equations $\delta S/\delta\phi = 0$ and $\delta S/\delta\rho = 0$. The first of these equations is a continuity equation, $\partial_t\rho + \nabla(\rho\mathbf{u}) = 0$ with $\mathbf{u} = \hbar\nabla\phi/m_B$. It can be easily solved in the spherically symmetric case yielding $\mathbf{u} = (\hat{\mathbf{r}}/r^2\rho)\int_0^r dr' r'^2 \partial_t\rho$. In terms of single variable ρ the action can be cast in the form

$$S = 4\pi\int dt dr r^2 \left[\frac{m_B}{2\rho}\left(\frac{1}{r^2}\int_0^r dr' r'^2 \partial_t\rho\right)^2 + \frac{\hbar^2(\nabla\rho)^2}{8m_B\rho} + E(\rho)\right]. \quad (3)$$

Evaluation of the extremum of S in the two cases of interest, i.e., near the line of the phase transition (at point X in Fig. 1a) and near the absolute instability line (at point Y), has been formally carried out in Ref. [3]. In the former case the solution can be parameterized as $\rho(r,t) \approx \rho_0\theta[r - R(t)]$ (the thin wall approximation), where $R(t)$ is the the radius of the critical droplet and ρ_0 is bosonic density of the mixed phase as before. Within such an approximation the action S can be formulated in terms of $R(t)$ as

$$S_X = 4\pi\int dt \left[\frac{m_B\rho_0}{2}R^3(\partial_t R)^2 + \sigma R^2 - \frac{\rho_0\Delta\mu}{3}R^3\right], \quad (4)$$

where the effective surface tension coefficient is $\sigma = \sqrt{\hbar^2/2m_B}\int d\sqrt{\rho}\sqrt{E(\rho)}$ and for $\Delta n_F/n_F^0 \ll 1$ we have $\Delta\mu = \lambda_{BF}K\Delta n_F$, with $K = [\frac{2}{3}(n_F^{0\,2/3} + n_B)^{3/2} - n_B n_F^{0\,1/3} - n_F^0]/n_B n_F^{0\,1/3}$, where n_B and n_F^0 are dimensionless as in Fig. 1a (n_B varies between 0 and 25/16). Evaluating the surface tension coefficient according to Eq. (1) and extremizing the action S_X, one obtains [11]

$$\ln\Gamma_X/\Gamma_0 = -0.0056\frac{n_B^{11/2}}{g_B K^{7/2}}\left(\frac{n_F^s}{\Delta n_F}\right)^{7/2}. \quad (5)$$

Precise evaluation of coefficient Γ_0 lies out of the scope of present calculations. It can be estimated, however, as $\Gamma_0/V \sim \omega_0/l^3$, where ω_0 is an "attempt" frequency. From the uncertainty principle $\omega_0 \sim \hbar/2m_B l^2$ and thus $\Gamma_0/V \sim \hbar/m_B l^5$.

As expected the tunneling exponent, i.e. the right-hand side of Eq. (5), is singular in the degree of metastability Δn_F and diverges as $\Delta n_F^{-7/2}$ [3]. Equation (5) also indicates that the rate of nucleation is exponentially small in the dilute limit, i.e., for $g_B \ll 1$. Note that appearance of the dimensionless boson density n_B in the numerator in Eq. (5) does not fix this problem, since the thin wall approximation (nucleation) requires sufficiently high energy barrier, e.g. Fig. 1(b,c), which is not the case when $n_B \ll 1$. However, due to the smallness of the numerical coefficient in the right-hand side of Eq. (5) one can hope that quantum nucleation is observable in sufficiently strongly coupled systems (which are presently realizable with the use of Feshbach resonance). Indeed, for $g_B \sim 0.1$, $n_B \sim 0.4$, and $\Delta n_F/n_F^s = 0.15$, the coefficient $K \sim 0.27$ and the tunneling exponent is ~ -27. For the same parameters and $a_{BB} \sim 20$ a.u., Γ_0/V can be estimated to be $\sim 10^{11} s^{-1}\mu m^{-3}$, which yields nucleation rate $\Gamma_X/V \sim 1\ s^{-1}\mu m^{-3}$.

Let us now evaluate the rate of transitions near the absolute instability of the mixed phase (at point Y in the phase diagram in Fig. 1a). Since the energy barrier in $E(\rho)$ is now relatively small and $E(\rho_0) \gg E(0)$, see Fig. 1c, one should pay attention only to the vicinity of the metastable minimum at ρ_0. Expanding action in Eq. (3) in $\delta\rho$, $\rho = \rho_0 + \delta\rho$, and retaining the second and the third order terms (in $\delta\rho$) in potential energy $E(\rho)$ and only the second order terms in the kinetic energy (the third order kinetic terms contain gradients and thus are small compared to the the third order potential terms in the limit of diverging coherence length near the point of absolute instability) one obtains

$$S_Y = 4\pi\int dt dr r^2 \left[\frac{m_B}{2\rho_0}\left(\frac{1}{r^2}\int_0^r dr' r'^2\partial_t\delta\rho\right)^2 + \frac{\hbar^2}{8m_B}\frac{(\nabla\delta\rho)^2}{\rho_0} + a\delta\rho^2 + b\delta\rho^3\right], \quad (6)$$

where

$$a = \frac{2\pi\hbar^2 a_{BB}}{3m_B}\left(1 - \frac{n_F}{n_F^s}\right);\ b = \frac{\hbar^2 a_{BF}^5 m_B}{3a_{BB}m_F^2}\left(1 + \frac{m_F}{m_B}\right)^5.$$

The extremum of S_Y is difficult to evaluate exactly. However, by introducing dimensionless variables $x = r\sqrt{8m_B\rho_0 a}/\hbar$, $\tau = 4\rho_0 a t/\hbar$, and $p = \delta\rho b/a$, the action S_Y can be rewritten as $const \times s_Y$, where $s_Y[p(x,\tau)]$ is a parameter-independent functional, the extremum of which is a c-number. Its value can be estimated by variational ansatz $p = -p_0\exp(-\alpha x^2 - \beta\tau^2)$, where α, β and p_0 are variational parameters. Upon a straightforward calculation one obtains

$$\ln\Gamma_Y/\Gamma_0 = -\frac{0.324}{g_B n_B^2}\left(1 - \frac{n_F}{n_F^s}\right)^{1/2}, \quad (7)$$

Again we see that tunneling exponent is controlled by the inverse boson gas parameter g_B. The exponent vanishes when fermion density n_F reaches value n_F^s, where the effective energy barrier disappears, see Fig. 1c. In this respect Eq. (7) is similar to results on macroscopic quantum tunneling (MQT) in systems of trapped bosons with attractive interactions [12], but with an important distinction: unlike in the latter case, the height of the potential barrier and thus the tunneling exponent for the critical droplet are controlled not by the total number of particles in the trap but the local densities. Therefore, for sufficiently large numbers of particles in the trap the tunneling exponent can be fine-tuned with a desired accuracy, which makes it possible to observe the MQT rate in a well controlled and predictable regime.

We now consider effects of dissipation on the kinetics of the first order phase transitions. The Thomas-Fermi approximation utilized in the derivation of the effective potential $E(\rho)$ implies that fermions instantaneously adjust to the local variation of boson density. Therefore it is instructive to proceed beyond this approximation and evaluate the effect of the excitation of particle-hole pairs in the fermionic subsystem on the dynamics of the transition. This effect can be estimated by considering the second order frequency dependent correction (in boson density ρ) produced by the interaction $\lambda_{BF}\psi_F^\dagger\psi_F\rho$. The resulting contribution to the effective action can be cast in the form

$$\Delta S = \frac{\lambda_{BF}^2}{2\hbar}\int\frac{d\mathbf{q}}{(2\pi)^3}\frac{d\omega}{2\pi}\left(\frac{m_F^2\,|\omega|}{4\pi\hbar^2 q}+...\right)|\rho(q,\omega)|^2, \quad (8)$$

where the ω and $\mathbf{q}$ independent term (omitted above) have already been included in Eq. (1), as can be verified by expanding $E(\rho)$ to the order $O(\rho^2)$. Again we consider the two cases: near the phase transition and near the absolute instability. Utilizing the thin wall approximation, $\rho(r,t)\approx\rho_0\theta[r-R(t)]$, we obtain that near the line of the phase transition the action in Eq. (8) can be written in terms of the radius of the critical droplet as

$$\Delta S_X = \frac{\lambda_{BF}^2 m_F^2\rho_0^2}{16\pi^2\hbar^3}\,\mathcal{P}\int\frac{dtdt'}{(t-t')^2}\left\{R(t)^3R(t') \quad (9)\right.$$
$$\left.+R(t)R(t')^3+\frac{1}{2}[R(t)^2-R(t')^2]^2\ln\left|\frac{R(t)-R(t')}{R(t)+R(t')}\right|\right\}.$$

The first two terms in the right-hand side of Eq. (9) arise due to the restructuring of the fermionic density of states inside the droplet in the course of its expansion, while the last term can be viewed as coupling between droplet's surface and particle-hole excitation in Fermi sea. Exact evaluation of extremal action (4) with the correction (9) is difficult and therefore we use the variational technique to evaluate the tunneling exponent. A natural ansatz is $R(t)=R_0e^{-\alpha t^2}$, where the turning point R_0 and coefficient α are variational parameters . We find that correction due to ΔS_X strongly alters the tunneling exponent in the region $K\Delta n_F/n_F^s\ll\eta_{dis}=g_B^{2/5}n_B^{9/5}(m_F/m_B)^{8/5}$:

$$\ln\Gamma'_X/\Gamma_0\approx-0.04\frac{n_B^{32/5}}{g_B^{4/5}K^4}\left(\frac{m_F}{m_B}\right)^{4/5}\left(\frac{n_F^s}{\Delta n_F}\right)^4, \quad (10)$$

while in the opposite (nondissipative) limit $\Delta n_F/n_F^s\gg\eta_{dis}$ the tunneling exponent is given by Eq. (5). We see from Eq. (10) that the influence of dissipation on the dynamics of nucleation is significant for $m_B\le m_F$.

Near the absolute instability (for $n_F\to n_F^s$) the contribution of dissipation, e.g. Eq. (8), can be estimated by using the same variational ansatz as in derivation of Eq. (7). We find that the tunneling exponent acquires an additional term $\sim-(m_Fg_Bn_B^2/m_B)^{4/5}$ (the numerical coefficient in Eq. (7) does not change significantly when ΔS is taken into account). This term is independent of fermion density and is again controlled by the mass ratio m_F/m_B. Therefore for not too high fermion/boson mass ratio, it is of the order $g_B^{4/5}$ and thus dissipation does not significantly alter the dynamics of the phase transition (MQT) in the absolute instability region.

Finally we estimate the crossover temperature between thermal and quantum regimes for the transition dynamics in the two cases of interest. The thermal regime becomes effective when the energy gap between the exited and the ground state energies of the metastable mixture is of the order k_BT [13]. This energy difference is $\hbar\Gamma_0\sim\hbar^2/2m_Bl^2$. Near the phase transition curve it gives the relation $g_B^{2/3}n_B\sim T/T_c$, where T_c is the Bose-Einstein condensate transition temperature. Since we assume $T\ll T_c$ and $n_B\sim1$, the tunneling is clearly the dominant process of nucleation. Near the spinodal instability we obtain $g_B^{2/3}(1-n_F/n_F^s)\sim T/T_c$. In this case, as expected, thermal excitation energy bounds the coherence length $l\sim(1-n_F/n_F^s)^{-1/2}$ for which the transition is dominated by MQT mechanism.

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